

July 3, 2003

Edwin L. Mongan
Manager, Environmental Stewardship
E.I. du Pont de Nemours & Company, Inc.
1007 Market Street, DuPont 6082
Wilmington, DE 19898

Dear Mr. Mongan:

The Office of Pollution Prevention and Toxics is transmitting EPA's comments on the robust summaries and test plan for Hexanedinitrile Hydrogenated, high-boiling Fraction (Crude BHMT) posted on the ChemRTK HPV Challenge Program Web site on February 25, 2003. I commend E.I. du Pont de Nemours & Company, Inc. and Solutia, Inc. for their commitment to the HPV Challenge Program.

EPA reviews test plans and robust summaries to determine whether the reported data and test plans will provide the data necessary to adequately characterize each SIDS endpoint. On its Challenge Web site, EPA has provided guidance for determining the adequacy of data and preparing test plans used to prioritize chemicals for further work.

EPA will post this letter and the enclosed comments on the HPV Challenge Web site within the next few days. As noted in the comments, we ask that E.I. du Pont de Nemours & Company, Inc. and Solutia, Inc. advise the Agency, within 60 days of this posting on the Web site, of any modifications to its submission.

If you have any questions about this response, please contact Richard Hefter, Chief of the HPV Chemicals Branch, at 202-564-7649. Submit questions about the HPV Challenge Program through the "Contact Us" link on the HPV Challenge Program Web site pages or through the TSCA Assistance Information Service (TSCA Hotline) at (202) 554-1404. The TSCA Hotline can also be reached by e-mail at tsca-hotline@epa.gov.

I thank you for your submission and look forward to your continued participation in the HPV Challenge Program.

Sincerely,

-S-

Oscar Hernandez, Director
Risk Assessment Division

Enclosure

cc: W. Penberthy
M. E. Weber

**EPA Comments on Chemical RTK HPV Challenge Submission:
Hydrogenated Hexanedinitrile, High-Boiling Fraction (Crude BHMT)**

Summary of EPA Comments

The sponsors, E.I. du Pont de Nemours & Company and Solutia, Inc., submitted a test plan and robust summaries to EPA for hexanedinitrile hydrogenated, high-boiling fraction (crude BHMT, CAS No. 68411-90-5) dated February 11, 2003. EPA posted the submission on the ChemRTK HPV Challenge Web site on February 25, 2003. Data were also provided for purified BHMT (bis(hexamethylene)triamine, CAS No. 143-23-7), the main component of the mixture.

EPA has reviewed this submission and has reached the following conclusions:

1. Substance Identification. The sponsored substance, crude BHMT, reportedly has a variable composition that typically consists of approximately 50-70% BHMT, 20-35% oligomeric amines, 0-10% C₁₀ amines, 0-10% hexamethylenediamine, 0-10% caprolactam, 0-5% adiponitrile, 0-5% 6-aminocapronitrile, and "small amounts of related compounds." The submitter needs to further identify "20-35% oligomeric amines" with representative structures and typical percentages.
2. Physicochemical Properties. The data provided by the submitter for melting point, boiling point, vapor pressure, and water solubility are adequate for the purposes of the HPV Challenge Program. The octanol/water partition coefficient data for the neutral form of BHMT are adequate for the purposes of the HPV Challenge Program. However, the submitter needs to describe in more detail the basis for their calculated value for ionized BHMT.
3. Environmental Fate. The data provided by the submitter for photodegradation and fugacity are adequate for the purposes of the HPV Challenge Program. The submitter needs to provide measured ready biodegradation data on crude BHMT and pKa data on the major constituent.
4. Health Effects. Adequate data are available for acute, repeated-dose, reproductive, and genetic toxicity endpoints on crude BHMT for the purposes of the HPV Challenge Program. The submitter needs to conduct a combined reproductive/developmental toxicity study on crude BHMT.
5. Ecological Effects. The submitted fish study is inadequate. The fish test needs to be added to the proposed aquatic toxicity tests, and because crude BHMT is a variable mixture, EPA recommends that the most representative mixture be tested and its composition characterized. The submitted ECOSAR-predicted toxicity values for purified BHMT are not adequate to represent the complex and variable composition of the sponsored substance, crude BHMT.

EPA requests that the submitter advise the Agency within 60 days of any modifications to its submission.

EPA Comments on the Crude BHMT Challenge Submission

Test Plan

Physicochemical Properties (melting point, boiling point, vapor pressure, partition coefficient and water solubility).

The data provided by the submitter for melting point, boiling point, vapor pressure, and water solubility are adequate for the purposes of the HPV Challenge Program.

Octanol/water partition coefficient. The octanol/water partition coefficient data for the neutral form of BHMT are adequate for the purposes of the HPV Challenge Program. However, EPA was unable to derive the submitter's value of -0.63 for the ionized form of BHMT. Instead, EPA calculated a value of

-0.14 using the SMILES notation NCCCCCNCCCCCN(H)(H)(H). The submitter needs to provide the SMILES notation of the ionized form of BHMT used in their calculation and verify their estimate.

Environmental Fate (photodegradation, stability in water, biodegradation, fugacity).

The data provided by the submitter for photodegradation and fugacity are adequate for the purposes of the HPV Challenge Program.

Stability in Water. EPA agrees that hydrolysis is not expected. However, because dissociation will occur, the submitter should provide a pK_a determination for at least BHMT itself using OECD TG 112.

Biodegradation. The submitter did not provide any biodegradation data for the crude BHMT but supplied biodegradation data for BHMT-HP Polyamine (purity >92 % by wt), following OECD Guideline 301 D, which indicate that it is readily biodegradable. The submitter concludes that crude BHMT is also readily biodegradable. However, because the biodegradation results were obtained from a purified BHMT, the data may not adequately reflect the biodegradation of the crude BHMT, which has 30 to 50% of other compounds. The submitter needs to provide measured ready biodegradation data on crude BHMT following OECD Guideline 301.

Health Effects (acute toxicity, repeated-dose toxicity, genetic toxicity, and reproductive/developmental toxicity).

Adequate data are available for acute, repeated-dose, reproductive, and genetic toxicity endpoints on crude BHMT for the purposes of the HPV Challenge Program. The submitter needs to conduct a combined reproductive/developmental toxicity study on crude BHMT.

Repeated-dose toxicity. The submitter needs to include the histopathologic examination of the reproductive organs of both sexes in the robust summaries for the 13-week gavage and inhalation studies.

Developmental toxicity. The submitted study is not adequate because no maternal toxicity was observed at 250 mg/kg/day, the highest dose tested. The submitter needs to conduct a combined reproductive/developmental toxicity study on crude BHMT following OECD TG 421 to adequately address this endpoint.

Ecological Effects (fish, invertebrates, and algae).

The submitted 48-hour static study on purified BHMT in *Leuciscus idus* is inadequate because the study duration was 48 rather than 96 hours, and the test substance was not neutralized prior to testing. The submitted predicted toxicity values for purified BHMT alone using ECOSAR do not account for the complex variable composition of the sponsored substance, crude BHMT. Therefore, the fish test needs to be included in the proposed aquatic toxicity testing.

Because the crude BHMT is a variable mixture, EPA recommends that the most representative mixture be tested and its composition characterized.

Specific Comments on the Robust Summaries

Health Effects

Information on the composition of the test material was not provided for some of the study summaries.

Followup Activity

EPA requests that the submitter advise the Agency within 60 days of any modifications to its submission.